ARKIV FÖR FYSIK Band 3 nr 21

Read 6 December 1950

Examination of the resolving power of the diffraction grating

By Erik Hulthén and Ulla Uhler.

With 12 figures in the text

Part I of this investigation describes a photographic and an electric method of determining the resolving power of spectroscopic instruments. The photographic method is performed with a plateholder which can be moved in measurable steps by a micrometer across the beam of the focal plane. The minimum step necessary for resolution of sharp iron lines thus gives the practical resolving power, the spectroscopic purity, of the instrument. — To avoid the difficulties from photographic blackening factors it is preferable to record the lines electrically with linear response (photomultipliers). The splitting of the spectral images into two components is here performed either by using a double-slit at the entrance of the spectrograph or by a double-slit placed in the focal plane in front of the photomultiplier, one slit movable towards the other by a micrometer. The photomultiplier here scans the spectrum. Two large concave gratings were examined.

Part II treats the Rayleigh criterion for the spectroscopic resolving power in cases where the grating is screened by a system of vertical strips. The amplitude-defects thus impressed on the grating give rise to ghosts situated symmetrically around the principal line. The improvements of the resolving power of the screened grating are discussed.

Part I

At the end of his now so famous paper on the resolving power of optical instruments, written in 1880, Lord Rayleigh (1) wishes:

"that the spectroscopists in possession of powerful instruments would compare their actual performances with those of which they are theoretically capable. A carefully arranged succession of tests of gradually increasing difficulty, like those applied to telescopes, would be of especial value."

Our examination is a rather late contribution along these lines of testing the properties of the diffraction gratings.

The resolving power of a spectroscopic instrument is generally defined as the ratio $\lambda/\delta\lambda$, where $\delta\lambda$ is the smallest wave-length difference between two spectral lines which the instrument is capable of separating. According to the Rayleigh criterion of optical resolution, the lines are resolved when their

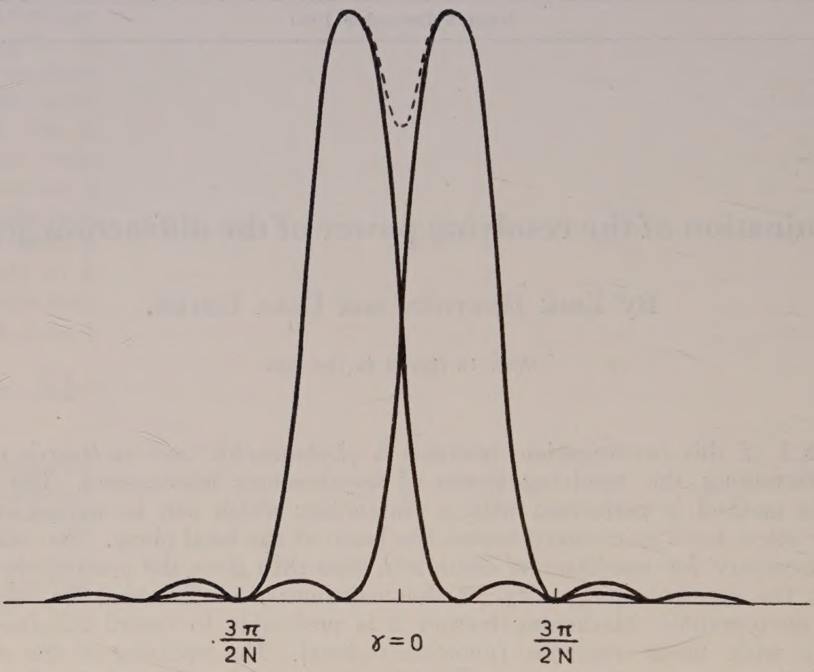

Fig. 1. The Rayleigh criterion for optical resolution.

principal images coincide with their first diffraction minima as shown in Fig. 1 According to the phase factor $\frac{\sin^2 \beta}{\beta^2}$ governing the intensity-distribution of these images, the outline of the doublet will be separated by an intensity minimum 81 % of that of the principal maxima. For an exhaustive discussion regarding other numerous suggestions which have been proposed from time to time as alternatives to the RAYLEIGH criterion we refer to a paper by RAMSAY, CLEVELAND and KOPPIUS (2).

The application of the Rayleigh criterion implies that the spectral lines are strictly monochromatic and that the slit of entrance is infinitely narrow. As these conditions can never be realized, our task is limited to a determination of the practical resolving power, the so-called spectroscopic purity, P, of the instrument. This being the case, P will here be defined in the same way as the resolving power, i.e. in correspondence to an intensity minimum, 81 % of that for the principal maxima of the doublet. It is evident that such determinations should be performed under conditions in close agreement with those holding for the ideal case.

Several proposals have been made about how to determine the spectroscopic resolving pover, e.g. by observing narrow doublets in the iron spectrum or in the absorption spectrum of iodine at room temperature and so on. None of these proposals, however, is free from objections, the separation of a given doublet rarely coinciding exactly with the case under consideration. A direct statement of the resolving power according to the Rayleigh criterion also requires the doublet components to be of equal intensity. These demands are, however, fulfilled by the following simple methods.

A region of the iron spectrum, containing sharp and suitable lines is photographed on a plateholder which can be moved by a micrometer across the beam in the focal plane. A series of double exposures is made with the plateholder moved in accurately measured steps. The minimum step, necessary for resolution, is determined and the result is stated in wave-length units and purity. To avoid the difficulties from photographic blackening factors and physiological contrast-phenomena it is preferable to record the lines electrically with linear response (photomultipliers). The splitting of the spectral image into two components is here performed either by using a double-slit at the entrance of the spectrograph or by a double-slit placed in the focal plane in front of the photomultiplier, one slit movable towards the other by a micrometer. The entire instrument here scans the spectrum.

Both of these methods, the photographic one and the electrical recording method, have their advantages and disadvantages. The former is experimentally very simple, but its results are highly dependent upon the time of exposure, the grain-size of the emulsion and so on. The electrical recording is preferable on account of its linear response, but there are some difficulties in adjusting the double slit parallel to the spectral line which will be discussed in detail below. The nature of these difficulties is indicated by the fact that the distance between the two slits in the case corresponding to the Rayleigh criterion, amounts to just a few microns. The photographic method does not offer similar difficulties.

The spectroscopic resolving power is ultimately related to the intensity distribution of the spectral image produced by the instrument. It might therefore seem most directly or spontaneously to record the outline hereof, as obviously the Rayleigh criterion according to figure 1 corresponds to the linewidth given at 40.5 percent of its maximal amplitude of intensity. Determinations of this kind, however, require recording devices of high stability and were found to be less sensitive than the double-slit method used by us.

All exposures and recordings have been carried out with a water-cooled hollow cathode of iron, which at low currents gives very sharp iron lines. At high currents the lines become noticeably broader, decreasing the spectral purity. Two large concave gratings, interchangeable in the same Eagle-mounting, have been the objects of our examination. The first grating mentioned here was ruled on speculum metal in ROWLAND's machine in 1889. This grating has been aluminized here and has a ruled surface of $2'' \times 5\frac{3}{4}''$ with 20 000 lines to the inch, corresponding to 115 000 lines in all. The other grating, ruled on aluminized pyrex by Professor R. W. WOOD in 1939, has a ruled surface of $2\,{}^1/_4'' \times 5\,{}^1/_2''$ with 30 000 lines to the inch, corresponding to 165 000 lines in all. Both gratings have a radius of curvature of 21′ (640 cm). The entrance-slit width, s, is determined according to the general condition

$$s = \lambda / \Phi \tag{1}$$

where Φ is the angular aperture of the grating. In our case this slit width is about 0.02 mm. Fig. 2 shows how the electrically recorded intensity of a line varies with the slit-width (3).

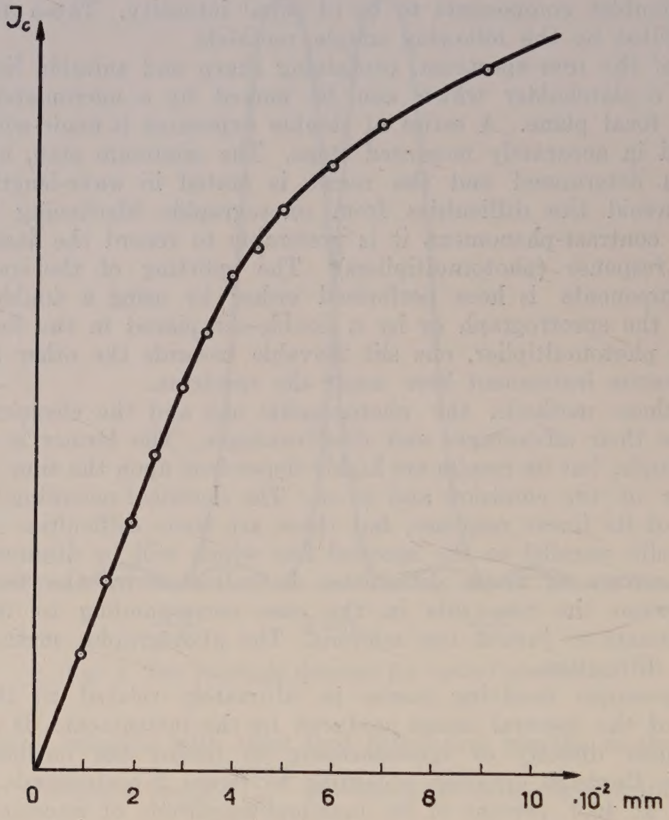

Fig. 2. Electrical recording of the line intensity at varying slit-widths.

The photographic method

The photographic recording was performed with a small plateholder movable in measurable steps of 2 microns along the focal plane of the spectrograph. This displacement is controllable even in darkness through the audible clicks of the steps. Fig 3a reproduces an exposure of the region around λ 3 000 Å of the iron spectrum, and figure 3b shows an enlarged picture of the doublet separation of one of these lines. The spectroscopic purity is visually estimated from the critical separation d_0 of the doublets, marked by the arrow in Fig. 3b. As a great number of lines is accessible for this estimation it is always easy to choose among those properly exposed. Some d_0-values, given in microns in Table 1, comprise our determinations of the three first orders in the Wood grating. It should be emphasized that the corresponding slit-widths have been chosen in accordance to (1) and independently of the spectral order under consideration. Thus the slit-width at 6 000 Å in the first order was twice that of the slit-width at 3 000 Å in the second order. In spite of this the orders are discriminative with regard to their attainable degree of spectroscopic purity.

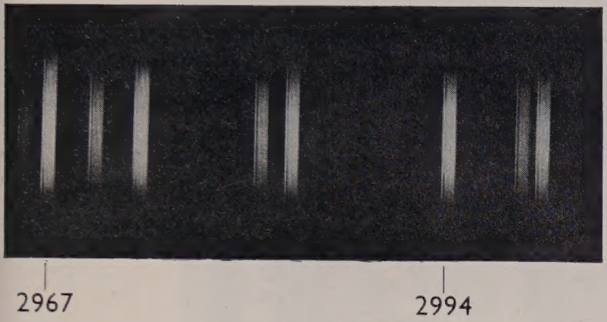

Fig. 3 a

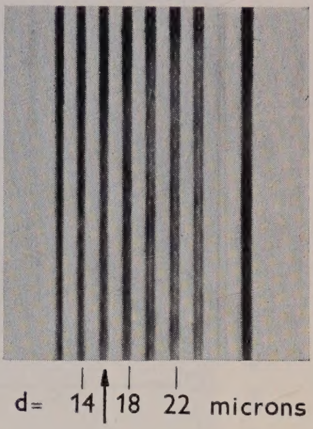

Fig. 3 b

The photographic doublet-method.

This remarkable fact is most directly seen from a comparison of the observed d_0-values with their theoretical values, derived from the relation:

$$d_{\text{theor.}} = L \cdot \Delta \lambda \tag{2}$$

Here L is the linear dispersion and $\Delta \lambda$ the theoretical limit of resolution in the Eagle mounting used by us. We are inclined to interpret the discriminating effect of the orders, whose percentual amounts are expressed in the last row of the table, as due to some imperfections or irregularities in the ruling of the grating.

Obviously no great weight can be attached to the absolute degree of purity, derived from the photographic doublet method here introduced. However, the critical d_0-values must be mutually rather compatible, as can be judged from

Table 1

$m\lambda$	d_0 microns	$d$theor.	$\frac{d_0}{d} \cdot 100$
1 × 3000	17	14	85
4300	26	21	80
6000	34	30	89
2 × 3000	23	15	66
3800	30	20	67
5500	26	19	73
3 × 3600	38	24	62

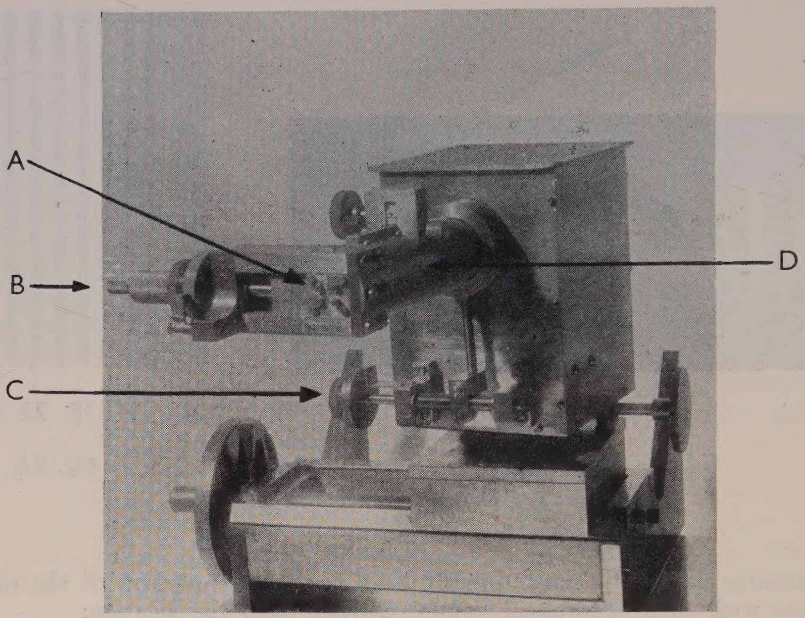

Fig. 4. The electrical recording instrument.

figure 3 b. In our view this method therefore deserves attention on account of its simplicity and the ease with which it may be applied and it might even be used as a rapid method of classifying the spectral lines according to their sharpness, pole-effects and so on.

The electrical method

The electrical recording method was performed with a double slit placed in front of the photomultiplier. Probably, this method would have been less troublesome in use, if the slit of entrance had acted as a double slit. This arrangement was, however, avoided, in order not to interrupt the precise settings of our Eagle-mounting.

The double slit, Fig. 4, is composed of one fixed and one movable slit, A, adjustable by a micrometer, B, similar to the one used in the photographic method. The parallelism of the slit and the spectral line is controlled by the screw C. The slits are fitted into a frame which is connected with the multiplier house by the adjustable tube D. The entire instrument is mounted on a comparator, the screw of which is driven by a synchronous motor, thus scanning a limited region of the spectrum. The recording instrument has been described by GLANSHOLM and KLEMAN (4).

When the double slit passes a spectral line, this is recorded by the slits in their proper turns. The slits have the same width as the entrance slit and they are so adjusted to the spectral line that they give equally large galvanometer deflections. The unavoidable light-openings arising between the two slit-jaws

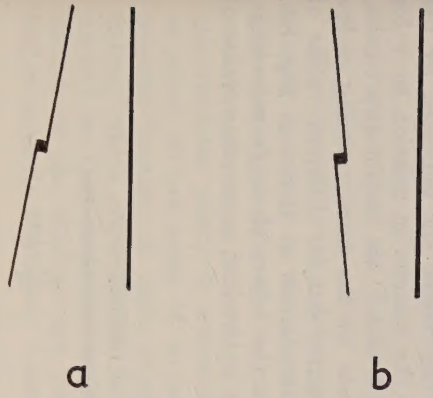

Fig. 5

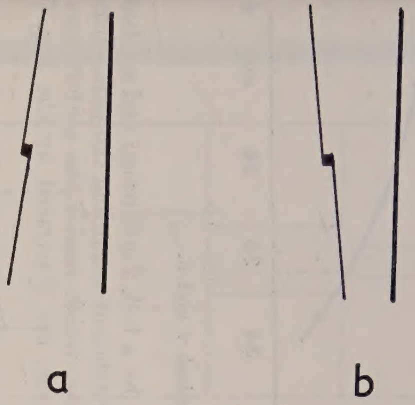

Fig. 6

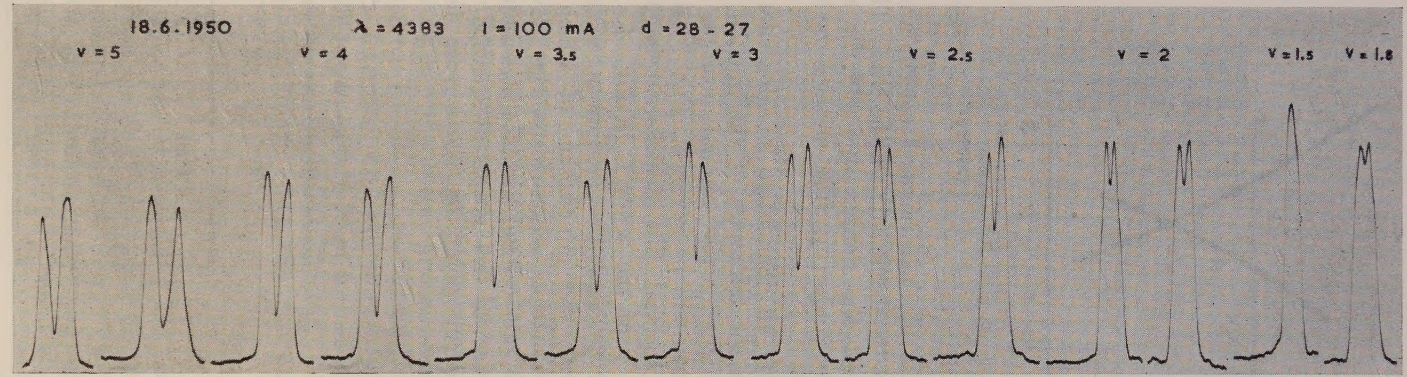

Fig. 7. Electrical recordings of λ 4383 at different inclinations of the double-slit.

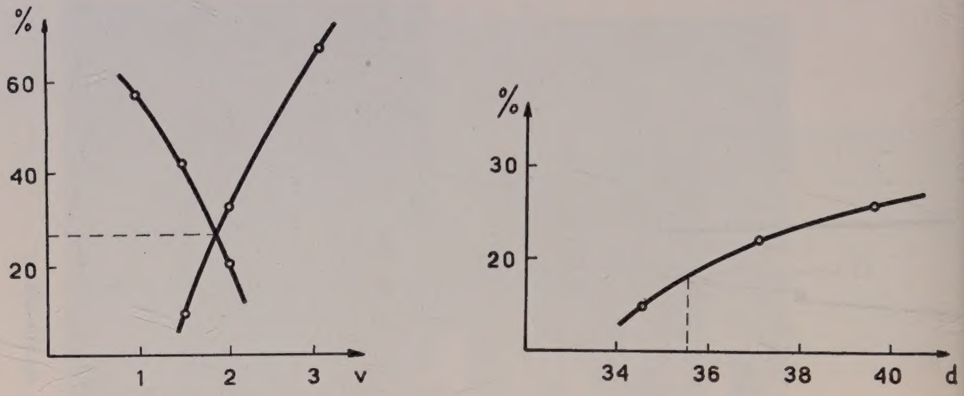

Fig. 8 a

Fig. 8 b

Cavity in percent plotted against v and d.

because of their rounded corners are screened by a lath 2 mm broad and applied across the back side of the slits. The high pretensions regarding the parallelism between the double slits and the spectral line, which render the performance of recordings by this method rather laborious, are illustrated by the Fig. 5 and 6.

Thus an inclination of the slits according to Fig. 5 a will obviously exaggerate the minimum of the doublet, while that of 5 b will smooth it down. By interchanging the mutual position of the slits, as shown in Fig. 6 a, b, these relations will be reversed. Fig. 7 shows some forward and backward recordings of a spectral line at different inclinations of the double slit indicated by the index v of the screw C in Fig. 4. Recording the minima in relation to v for mutal positions of the slits according to Fig. 5 and 6, we obtain two curves, Fig. 8 a, the intersection of which corresponds to the correct setting of the slit-inclination. Such recordings have been carried out for different values of d, and the critical distance d_0 obtained by interpolation as shown in Fig. 8 b. The use of the graphical method will reduce the errors of single recordings, and every point on the curves in Fig. 8 a is obtained as a mean value of

Table 2

The Wood Grating, R = 165000.

$m\lambda$	d_0 microns	$d_{\text{theor,}}$	$\frac{d_0}{d} \cdot 100$
1 × 3440	27.8	16.6	59.6
4375	31.0	21.2	68.5
4383.5	29.8	21.3	71.5
5014	41.8	24.9	59.5
5615	41.8	28.1	68.5
2 × 4383	35.5	24.3	68.5

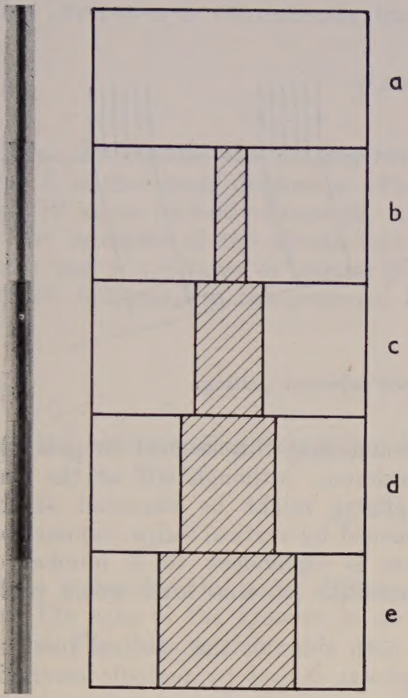

Fig. 9

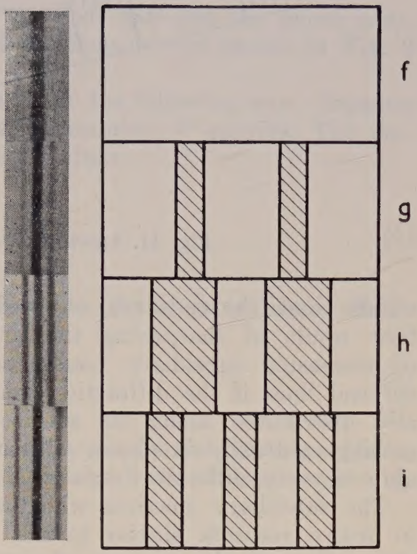

Fig. 10

Diffraction patterns of the screened grating.

the forward and the backward recordings of the line, seldom differing more than 5 % from each other.

The results of our determinations of the spectroscopic purity of the Wood grating according to the electrical recording method are given in Table 2 below. The observed values of the purity are here somewhat lower than those obtained with the photographic method (cf. Table 1). In the case of the Rowland grating the available purity is somewhat lower than for the Wood grating, amounting to about 60 per cents of its theoretical value. The lines investigated have been selected because of their relatively high intensity, and the spread in the P-values, which amounts to more than 5%, may, apart from focussing errors, depend on their imperfections in respect of symmetry and sharpness. Thus the humps of the doublet are rapidly smoothed down, when the current in the hollow cathode increases.

Part II

Lord Rayleigh, in his above cited paper, also investigated the effect of screening the central part of a rectangular section, expressing the intensity of the image by means of the Bessel functions of the first order. The diffraction phenomena showed a sharpening of the principal maximum, while the intensities of the subsidiary maxima increased disturbingly. Tentatively testing the case where portions of the rectangular section intermediate between the

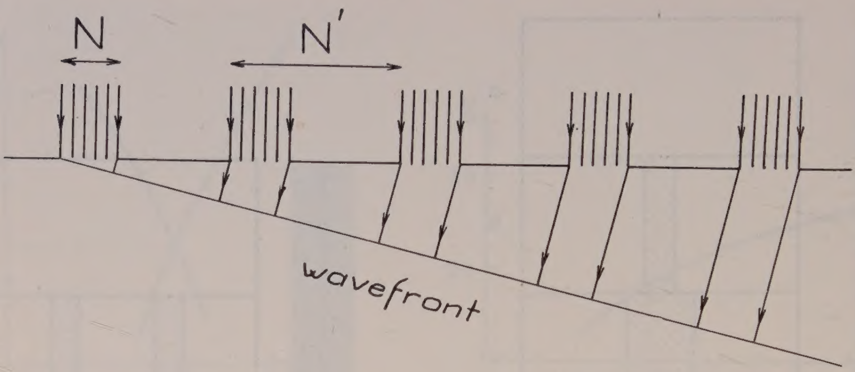

Fig. 11. Apertures and strips at the screened grating.

middle and the ends are screened off, he found that this seemed to give the best result of sharpening the principal maximum, although still at the cost of increasing subsidiary maxima. Similar effects might be expected at the spectral lines if the diffraction grating is screened by vertical strips, symmetrically distributed along its surface. This case is equivalent to a number of gratings mutually in phase, although a composition of this kind would probably be very difficult to realize.

The subsidiary maxima which appear on both sides of the spectral line are in many respects similar to the Rowland ghosts caused by periodic errors in the ruling of the grooves. In our case this periodicity is imposed upon the grating by screening it with a system of wires or paper strips.

The appearance of these artificially produced ghosts is shown in Fig. 9 and and 10, accompanied by their screening patterns. We will now calculate their position and intensity in relation to the principal line with help of Fig. 11.

Denoting the grating constant by σ and the corresponding coarse spacing of the screening pattern by a, the incident angle by i and the diffraction angles by θ and θ', we obtain for the principal line:

$$\sin i + \sin \theta = \frac{m\lambda}{\sigma}$$

m denotes the order of the spectrum and M is the order of the ghost line. Only those lines corresponding to $M = 1$ were strong enough to be seen here. For the ghost lines of the order M we have:

$$\sin i + \sin \theta' = \frac{m\lambda}{\sigma} \pm \frac{M\lambda}{a}$$

Thus

$$\sin \theta' - \sin \theta = \pm \frac{M\lambda}{a}$$

or

$$\theta' - \theta = \pm \frac{M\lambda}{a \cos \theta}$$

This expression is conveniently transformed into

$$\varDelta x = \pm \frac{M\sigma}{a} \cdot L\lambda \tag{3}$$

where $\varDelta x$ denotes the spacing between the principal line and the ghost lines, and L is the linear dispersion. The observed positions of the ghosts in Fig. 9 and 10 agree perfectly herewith.

The intensity of the ghosts may be calculated in the following way. Suppose there are p apertures or partial gratings, each containing N grooves. The amplitude belonging to the principal line may be written:

$$A_p = A_0 \cdot \sum_{u=0}^{Np} e^{i(\omega t + \mu \cdot 2\pi)} \tag{4}$$

and the corresponding expression for the amplitude of the ghost line is then

$$A_g = A_0 p \sum_{u=0}^{N} e^{i(\omega t + u\gamma)}, \tag{5}$$

where γ denotes the phase difference between adjacent partial gratings. Denoting the sum of the grooves in an aperture and behind its adjacent screen by N′ (cf. Fig. 11), we have

$$\gamma = \frac{2\pi}{N'} \cdot M \tag{6}$$

Squaring (4) and (5) and selecting the real or the imaginary part hereof, we obtain the following intensities:

$$I_p = A_p^2 = A_0^2 p^2 N^2 \tag{7}$$

$$I_g = A_g^2 = A_0^2 p^2 \frac{\sin^2 \dfrac{N\pi}{N'}}{\sin^2 \dfrac{\pi}{N'}} \approx A_0^2 p^2 \cdot \frac{N'^2}{M^2 \pi^2} \cdot \sin^2 \frac{N\pi M}{N'} \tag{8}$$

According to these notations, intensity of the principal line at the grating unscreened, will be:

$$I = A_0^2 p^2 N'^2, \tag{9}$$

and consequently

$$\frac{I_p}{I_0} = \left(\frac{N}{N'}\right)^2 \tag{10}$$

and

$$\frac{I_g}{I_0} = \frac{1}{\pi^2} \sin^2 \left(\frac{N\pi M}{N'}\right). \tag{11}$$

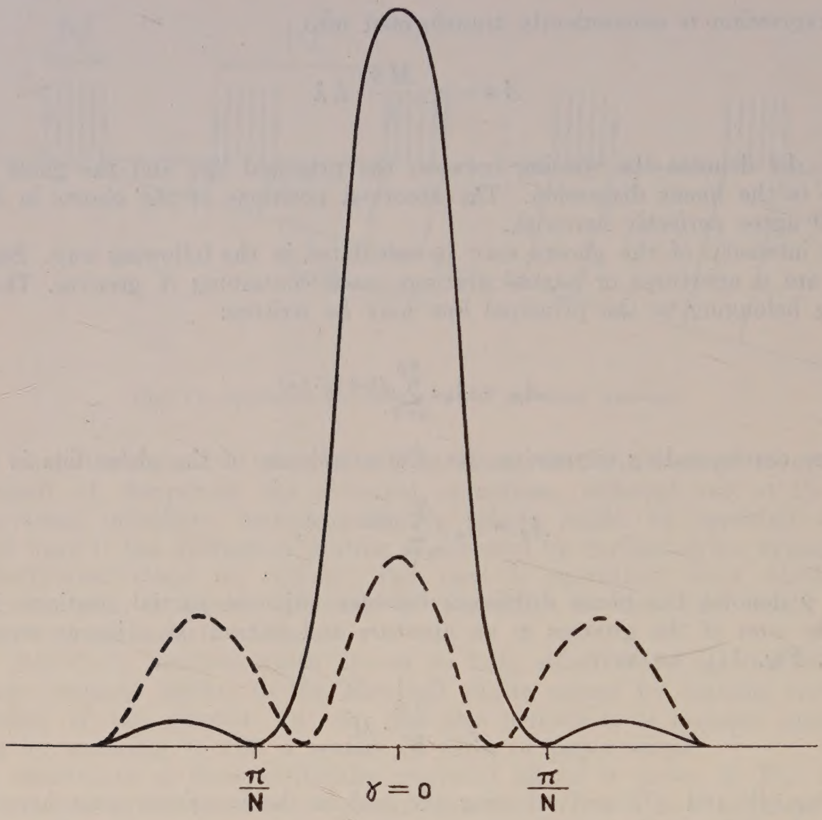

Fig. 12. The calculated intensity distribution (dotted curve) of the diffraction images exhibited by the gratings screened according to the pattern given in Fig 9e.

It therefore appears that the intensities of the ghost lines increases with the screening amount of the grating, reaching their maximum for $N' = 2N$, i.e. when screening the grating with wires or strips having the same widths as the apertures. Similarly all ghosts corresponding to even orders of M will then disappear.

According to (7), the intensity of the principal line decreases in proportion to the square of the illuminated width of the grating. But as the total intensity of the diffraction-patterns is reduced in proportion to the illuminated width of the grating, the excess of light-energy must fall upon the subsidiary maxima, i.e. the ghosts.

There seems to be an approximate agreement between the intensity relations derived above and those emerging from the Fig. 9 and 10.

A more detailed analysis of the intensity-distribution of the diffraction patterns shows that their sharpness may be considerably increased by screening the grating. This also emerges from the Fig. 9 and 10, and it is further illustrated by Fig. 12, which represents the calculated intensity-distribution corresponding to the case 9e, where half the grating surface is screened. The width of the principal line is here reduced to 2/3 of its original width, a fact which is easily derived from the condition holding for adjacent minima with the screening pattern here considered.

Thus it is possible by a suitable screening of the grating to increase its resolving power considerably, which is done, however, at expense of its intensity. By screening it with a fine wire gauze it is also possible to displace the ghost so far away from the principal line that regions wide enough for the study of single isolated line-groups e.g. the hyperfine structure of atomic lines and narrow bandheads are available. These studies will be continued.

We want to express our thanks to Fil. lic. BENGT KLEMAN and Mr. DANIEL GLANSHOLM for their valuable help and for their kindness to place at our disposal the photoelectrical apparatus.

REFERENCES: [1] Lord **Rayleigh,** Scientific Papers, Vol. 1, p. 459, Cambridge, University Press. — [2] **B. P. Ramsay, E. L. Cleveland** and **O. T. Koppius,** J. Opt. Soc. Am. **31,** 26 (1941). — [3] For a comparison with the theoretical case, see van **Cittert,** Zeitschrift f. Physik, **65,** 547 (1930). — [4] **D. Glansholm** and **B. Kleman,** Arkiv för Fysik, **2,** 20, 1950.

Tryckt den 11 augusti 1951

Uppsala 1951. Almqvist & Wiksells Boktryckeri AB